LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV122821\
Data File : VV024228.D
Acq On : 28 Dec 2021 19:10
Operator : SY/MD
Sample : M5233-11DL2 100X
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
GBCC9DL2

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.1 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR122721WMA.M
Title : TRACE VOA SFAM1.0

Signal : TIC: VV024228.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.108	16	21	33	rVB3	14226	16365	3.91%	0.392%
2	1.214	48	54	62	rBV	39501	41139	9.82%	0.986%
3	1.294	72	79	91	rVB2	386968	418891	100.00%	10.041%
4	1.356	92	98	104	rBV	42257	39821	9.51%	0.955%
5	1.417	104	117	133	rBV2	77318	181194	43.26%	4.343%
6	1.584	159	169	179	rVB2	109889	160705	38.36%	3.852%
7	1.819	236	242	253	rVB4	14700	23234	5.55%	0.557%
8	1.902	263	268	279	rVB	14209	18162	4.34%	0.435%
9	2.024	298	306	320	rVV	50265	74398	17.76%	1.783%
10	2.108	323	332	346	rVB	82796	124136	29.63%	2.976%
11	2.481	437	448	468	rBV3	15982	38099	9.10%	0.913%
12	2.577	468	478	491	rVB8	5729	11963	2.86%	0.287%
13	3.761	836	846	856	rBV7	2596	6125	1.46%	0.147%
14	3.899	878	889	916	rBV3	26859	91933	21.95%	2.204%
15	4.346	1013	1028	1053	rBV2	59432	152116	36.31%	3.646%
16	4.462	1055	1064	1075	rVB5	4755	9336	2.23%	0.224%
17	5.050	1225	1247	1256	rBV2	122443	302790	72.28%	7.258%
18	5.098	1257	1262	1284	rVB	79386	166518	39.75%	3.992%
19	5.224	1289	1301	1314	rVB3	7668	16946	4.05%	0.406%
20	5.616	1411	1423	1448	rBV	85520	180269	43.03%	4.321%
21	5.950	1516	1527	1539	rVB8	6879	14463	3.45%	0.347%
22	6.069	1551	1564	1583	rBV3	72023	148668	35.49%	3.564%
23	6.802	1785	1792	1803	rVB6	2688	4679	1.12%	0.112%
24	6.989	1840	1850	1865	rBV3	26601	48802	11.65%	1.170%
25	7.169	1899	1906	1916	rVB6	3323	5303	1.27%	0.127%
26	7.317	1940	1952	1967	rBV	144195	250483	59.80%	6.004%
27	7.391	1967	1975	1989	rVB	25857	46660	11.14%	1.118%
28	7.625	2035	2048	2060	rBV2	14855	27362	6.53%	0.656%
29	7.709	2063	2074	2085	rVB4	3599	7479	1.79%	0.179%
30	8.088	2178	2192	2224	rBV	133231	253237	60.45%	6.070%
31	8.420	2285	2295	2305	rBV4	5947	9885	2.36%	0.237%
32	8.854	2419	2430	2456	rBV	145009	245486	58.60%	5.884%
33	9.014	2469	2480	2498	rBV	53685	85769	20.48%	2.056%
34	9.140	2503	2519	2532	rBV	59361	100147	23.91%	2.401%
35	9.265	2546	2558	2561	rBV7	4076	5811	1.39%	0.139%
36	9.301	2562	2569	2587	rVB3	18003	32858	7.84%	0.788%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV122821\
Data File : VV024228.D
Acq On : 28 Dec 2021 19:10
Operator : SY/MD
Sample : M5233-11DL2 100X
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
GBCC9DL2

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.1 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR122721WMA.M
Title : TRACE VOA SFAM1.0

37	9.545	2636	2645	2657	rVB	32810	50768	12.12%	1.217%
38	9.863	2733	2744	2754	rBV7	3828	6331	1.51%	0.152%
39	9.931	2760	2765	2774	rVB3	4338	5627	1.34%	0.135%
40	10.217	2843	2854	2866	rBV	50685	80266	19.16%	1.924%
41	10.358	2890	2898	2909	rBV3	4403	7341	1.75%	0.176%
42	10.474	2926	2934	2945	rVB3	5427	7423	1.77%	0.178%
43	10.738	3009	3016	3026	rVB2	12945	19703	4.70%	0.472%
44	10.915	3059	3071	3087	rBV	12839	19907	4.75%	0.477%
45	11.249	3164	3175	3193	rVB	160737	248034	59.21%	5.946%
46	11.336	3193	3202	3212	rBV	23509	35203	8.40%	0.844%
47	11.526	3251	3261	3276	rVB	16401	27415	6.54%	0.657%
48	11.625	3280	3292	3314	rVB	158385	258711	61.76%	6.201%
49	12.017	3404	3414	3419	rBV4	4012	5984	1.43%	0.143%
50	12.111	3433	3443	3456	rVB8	6482	10064	2.40%	0.241%
51	12.725	3627	3634	3643	rBV5	2892	4768	1.14%	0.114%
52	12.882	3674	3683	3695	rVB5	8619	13551	3.23%	0.325%
53	13.506	3869	3877	3885	rBV	5808	9446	2.26%	0.226%

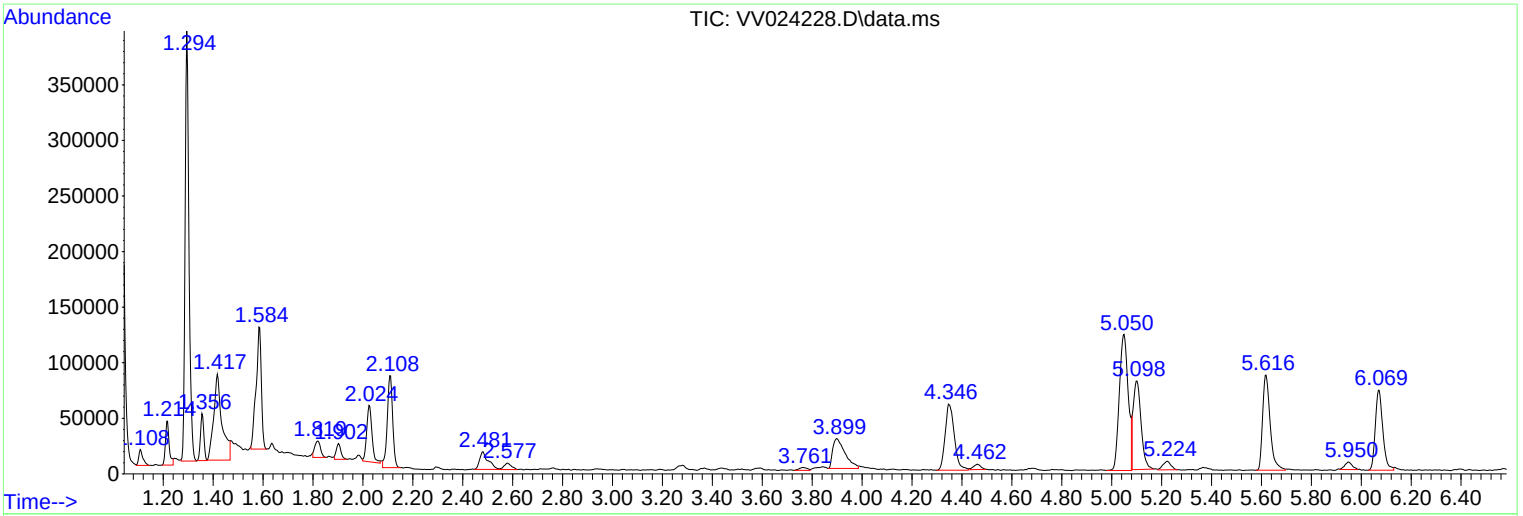
Sum of corrected areas: 4171774

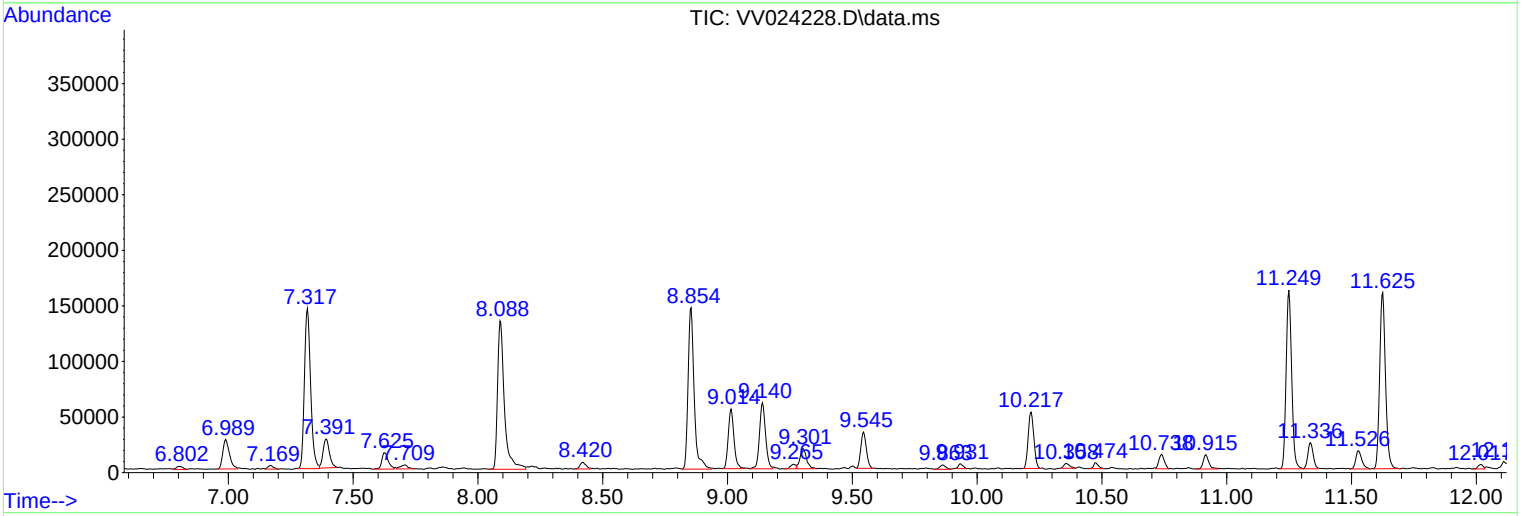
Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV122821\
Data File : VV024228.D
Acq On : 28 Dec 2021 19:10
Operator : SY/MD
Sample : M5233-11DL2 100X
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 25 Sample Multiplier: 1

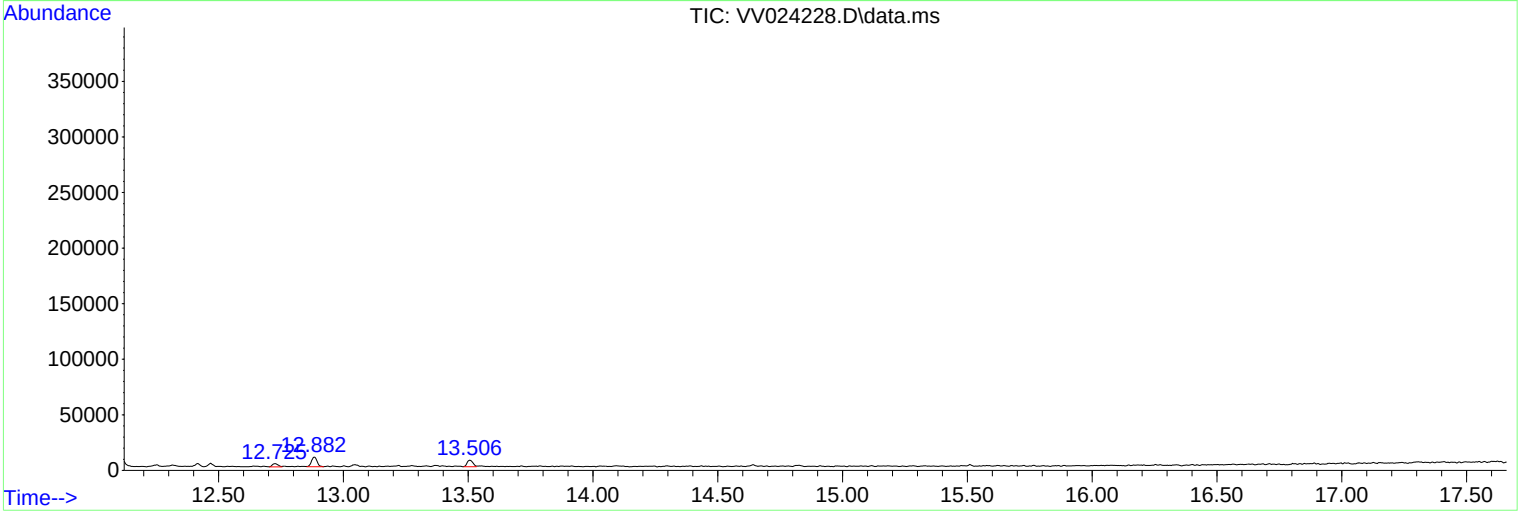
Instrument :
MSVOA_V
ClientSampleId :
GBCC9DL2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR122721WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P







Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV122821\
Data File : VV024228.D
Acq On : 28 Dec 2021 19:10
Operator : SY/MD
Sample : M5233-11DL2 100X
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
GBCC9DL2

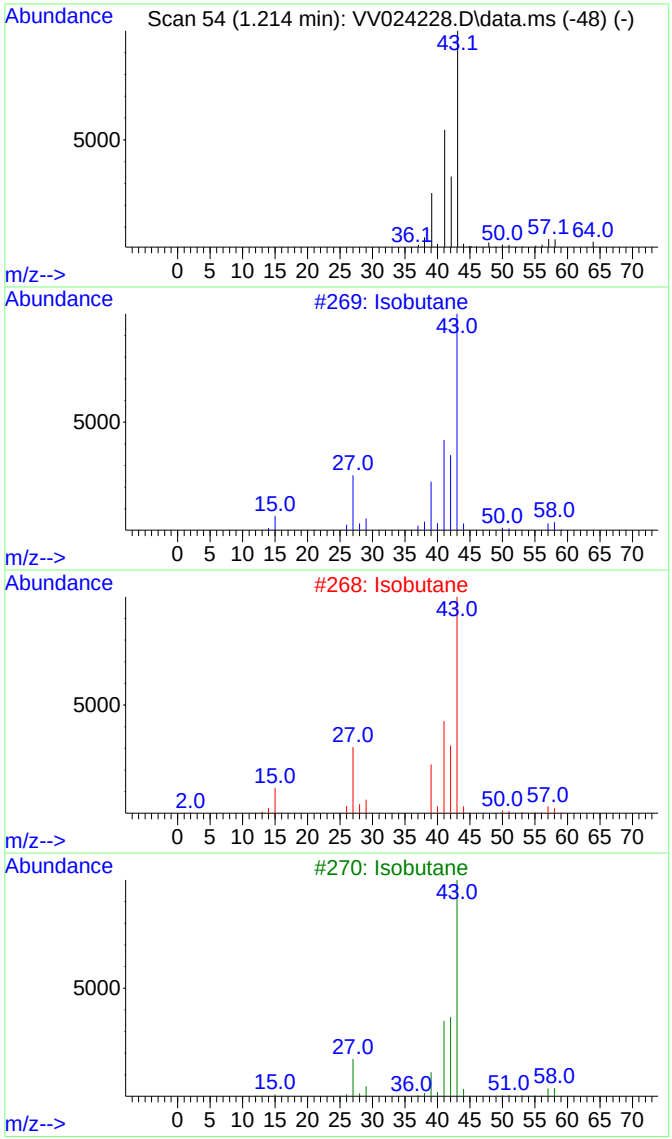
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR122721WMA.M
Quant Title : TRACE VOA SFAM1.0

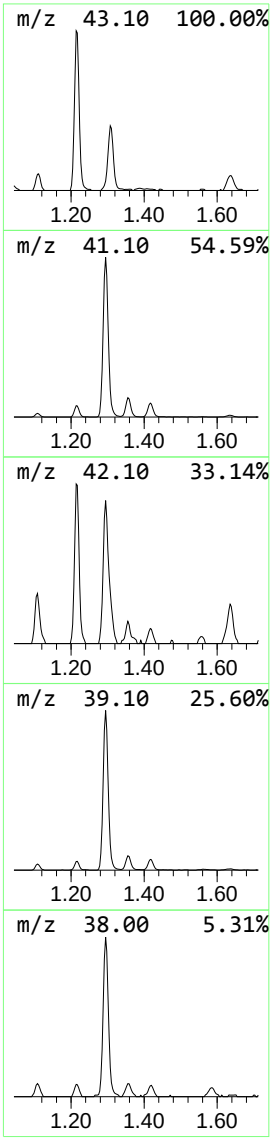
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.214	1.14 ug/L	41139	1,4-Difluorobenzene	5.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutane	58	C4H10	000075-28-5	50
2	Isobutane	58	C4H10	000075-28-5	50
3	Isobutane	58	C4H10	000075-28-5	42
4	Isobutyl nitrite	103	C4H9NO2	000542-56-3	23
5	Isobutane	58	C4H10	000075-28-5	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV122821\
Data File : VV024228.D
Acq On : 28 Dec 2021 19:10
Operator : SY/MD
Sample : M5233-11DL2 100X
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
GBCC9DL2

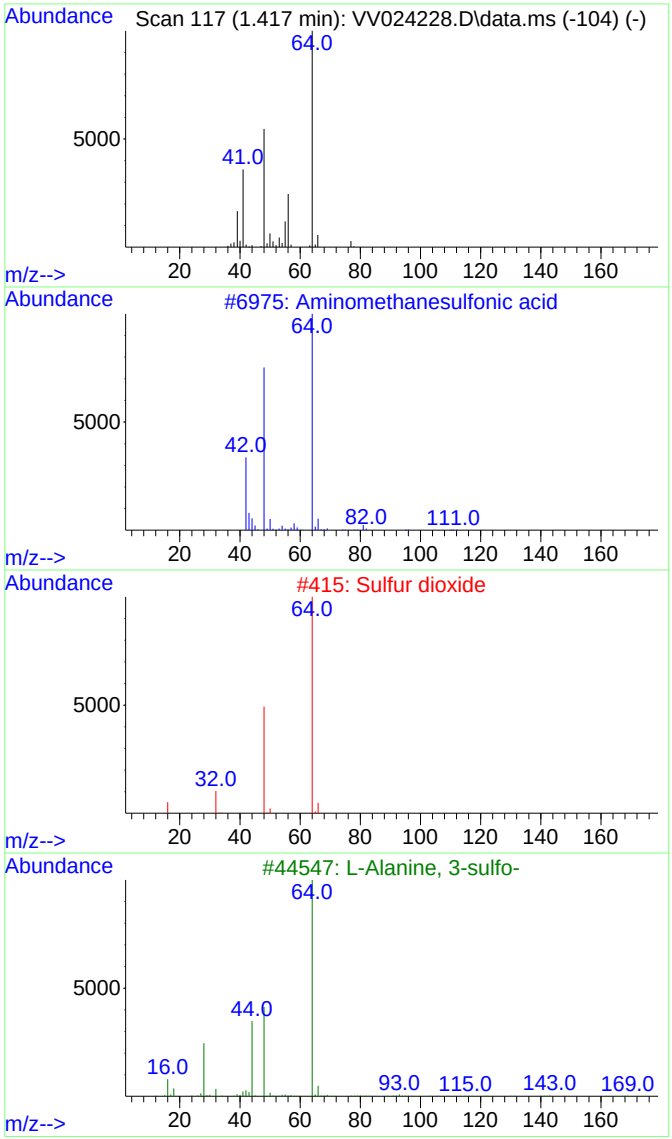
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR122721WMA.M
Quant Title : TRACE VOA SFAM1.0

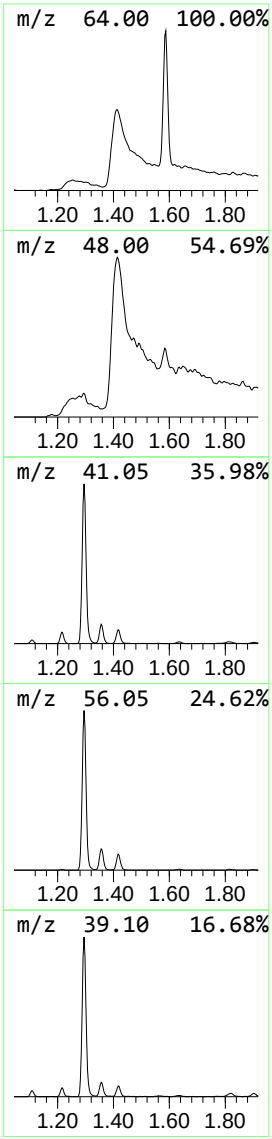
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Aminomethanesulfonic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.417	5.03 ug/L	181194	1,4-Difluorobenzene	5.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	78
2	Sulfur dioxide	64	O2S	007446-09-5	64
3	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV122821\
Data File : VV024228.D
Acq On : 28 Dec 2021 19:10
Operator : SY/MD
Sample : M5233-11DL2 100X
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
GBCC9DL2

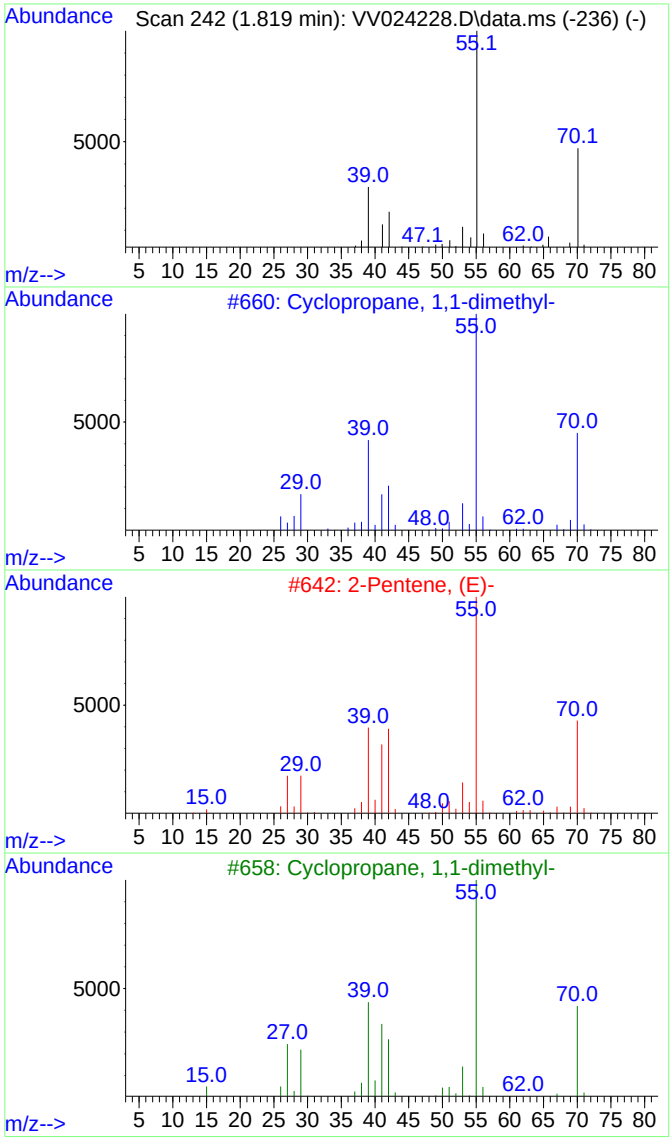
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR122721WMA.M
Quant Title : TRACE VOA SFAM1.0

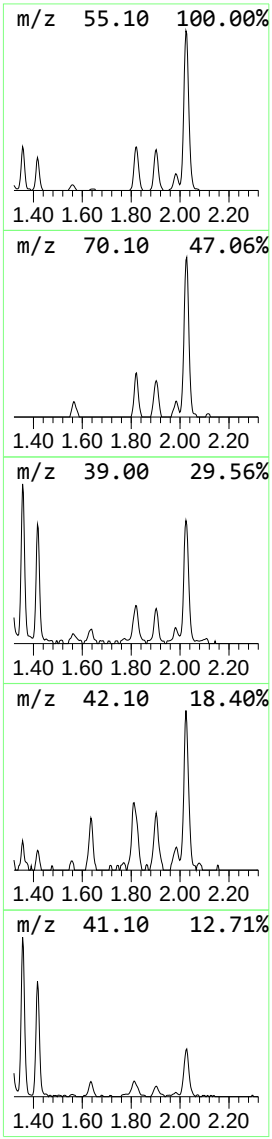
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 (DEL) Alkane: Cyclic1.819 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.819	0.64 ug/L	23234	1,4-Difluorobenzene	5.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	81
2	2-Pentene, (E)-	70	C5H10	000646-04-8	68
3	Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	64
4	2-Butene, 2-methyl-	70	C5H10	000513-35-9	64
5	2-Methyl-1-butene	70	C5H10	000563-46-2	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV122821\
Data File : VV024228.D
Acq On : 28 Dec 2021 19:10
Operator : SY/MD
Sample : M5233-11DL2 100X
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
GBCC9DL2

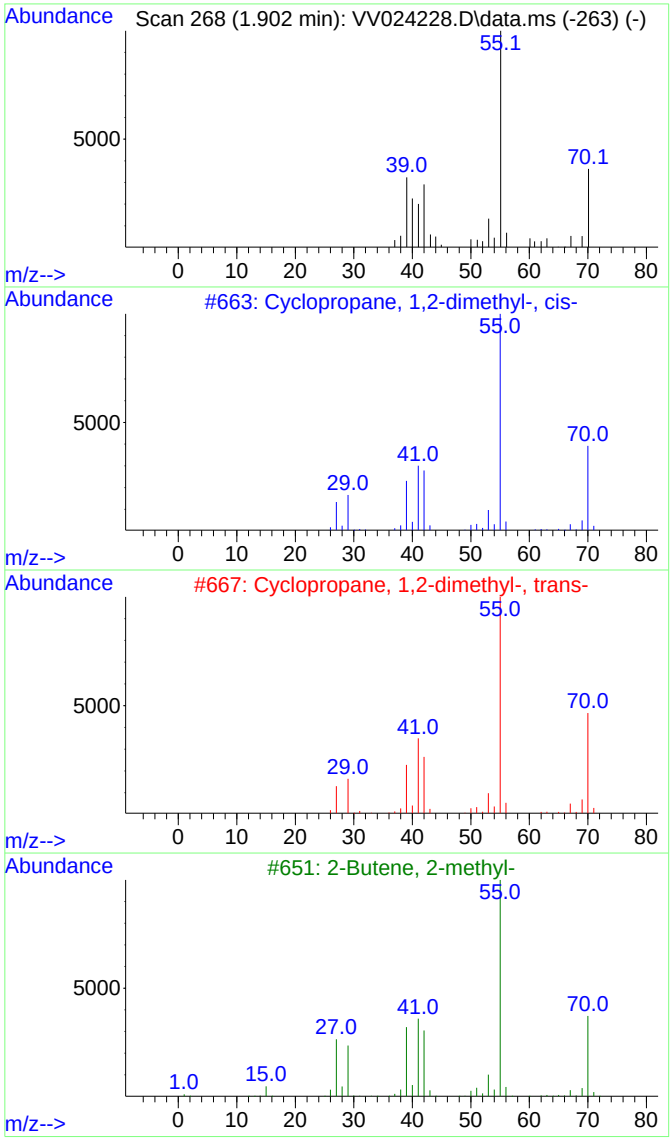
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR122721WMA.M
Quant Title : TRACE VOA SFAM1.0

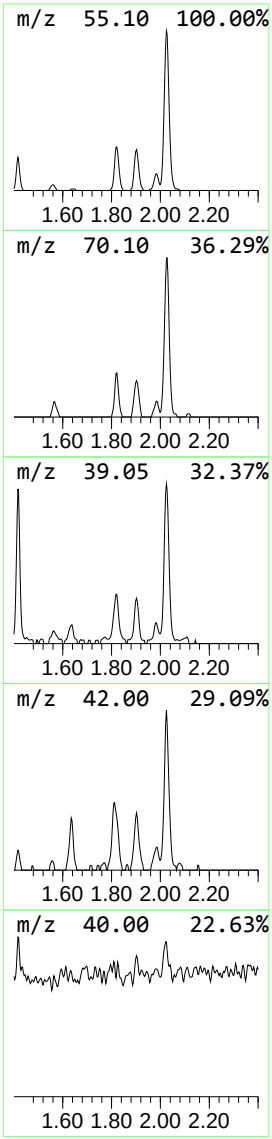
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 (DEL) Alkane: Cyclic1.902 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.902	0.50 ug/L	18162	1,4-Difluorobenzene	5.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	80
2	Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	80
3	2-Butene, 2-methyl-	70	C5H10	000513-35-9	80
4	1-Butene, 3-methyl-	70	C5H10	000563-45-1	80
5	2-Butene, 2-methyl-	70	C5H10	000513-35-9	72





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV122821\
Data File : VV024228.D
Acq On : 28 Dec 2021 19:10
Operator : SY/MD
Sample : M5233-11DL2 100X
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
GBCC9DL2

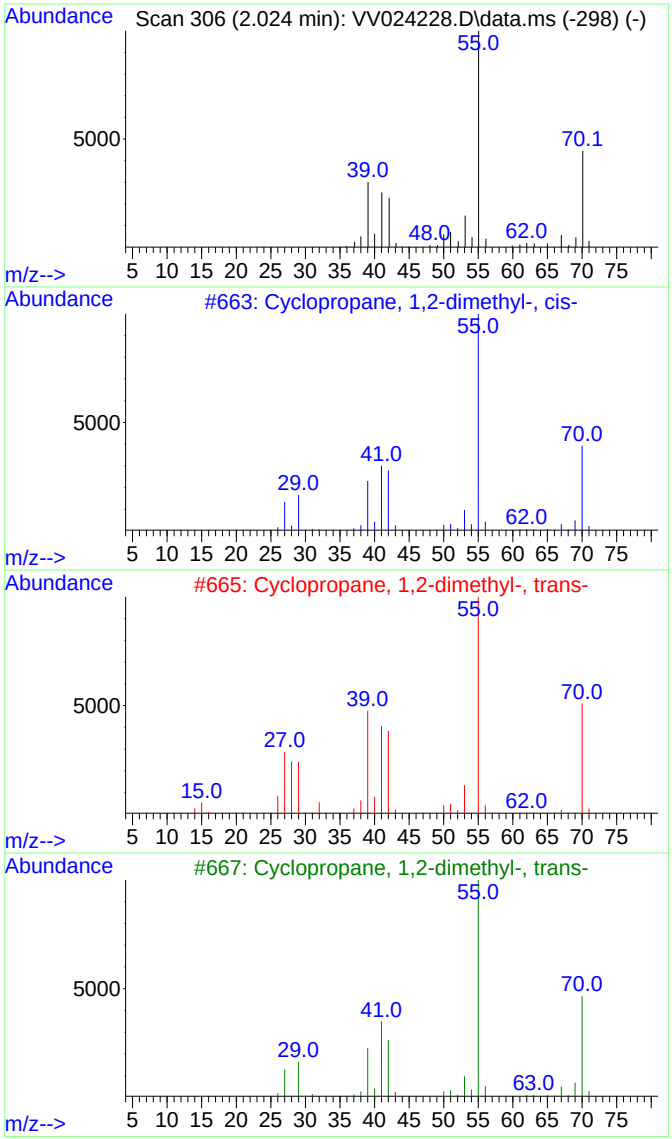
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR122721WMA.M
Quant Title : TRACE VOA SFAM1.0

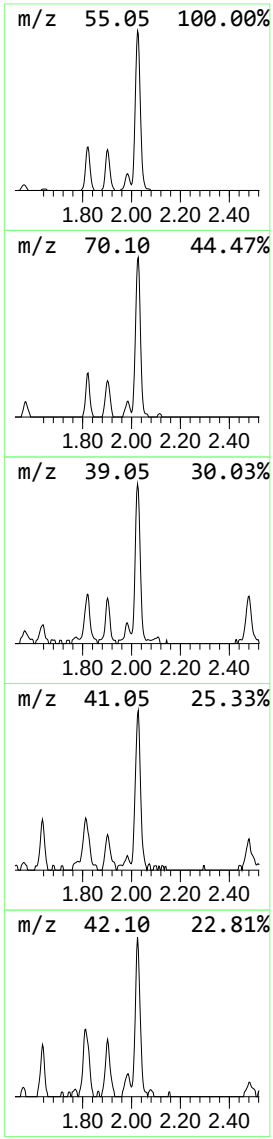
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 (DEL) Alkane: Cyclic2.024 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.024	2.06 ug/L	74398	1,4-Difluorobenzene	5.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	86
2	Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	83
3	Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	83
4	2-Butene, 2-methyl-	70	C5H10	000513-35-9	80
5	Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	80





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV122821\
Data File : VV024228.D
Acq On : 28 Dec 2021 19:10
Operator : SY/MD
Sample : M5233-11DL2 100X
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
GBCC9DL2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR122721WMA.M
Quant Title : TRACE VOA SFAM1.0

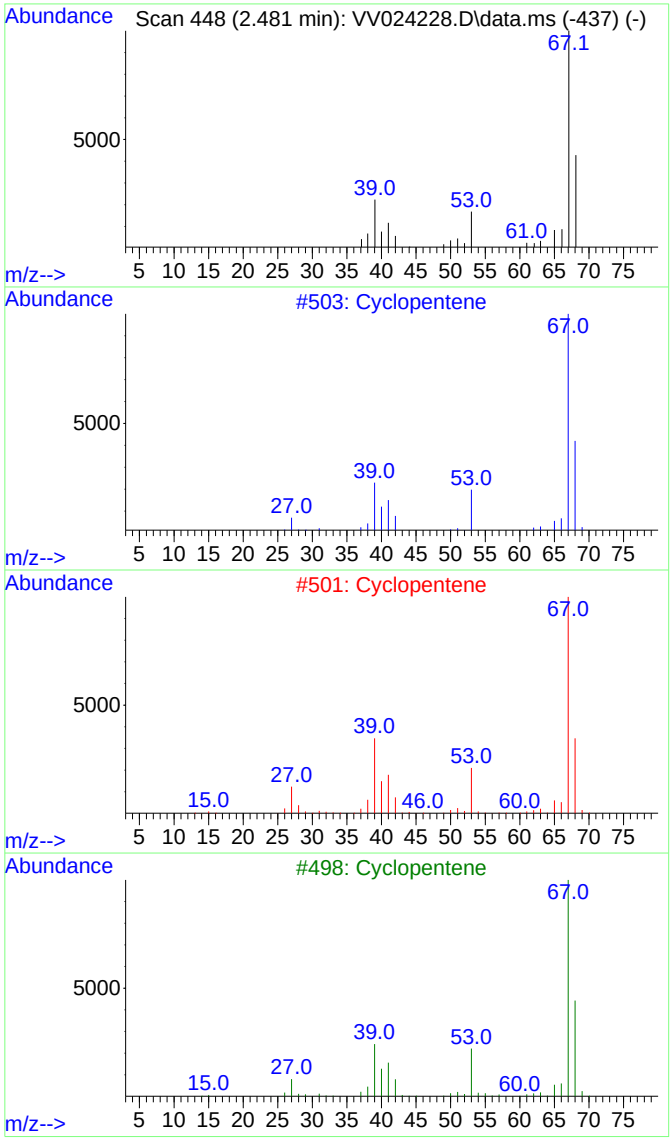
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

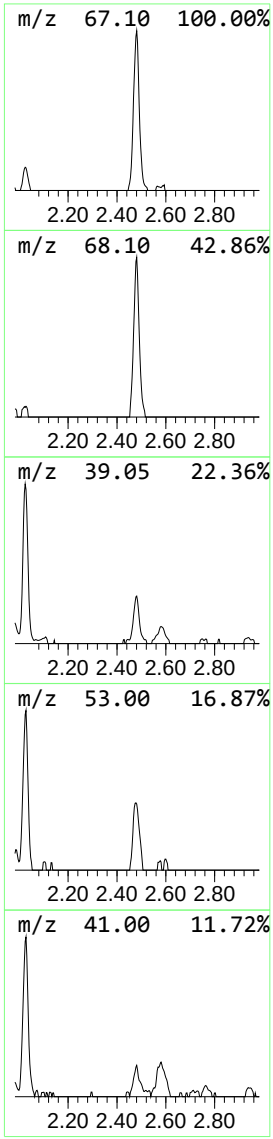
****

Peak Number 6 Cyclopentene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.481	1.06 ug/L	38099	1,4-Difluorobenzene	5.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentene	68	C5H8	000142-29-0	87
2	Cyclopentene	68	C5H8	000142-29-0	86
3	Cyclopentene	68	C5H8	000142-29-0	86
4	Cyclopentene	68	C5H8	000142-29-0	83
5	Cyclopentene	68	C5H8	000142-29-0	78





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV122821\
Data File : VV024228.D
Acq On : 28 Dec 2021 19:10
Operator : SY/MD
Sample : M5233-11DL2 100X
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
GBCC9DL2

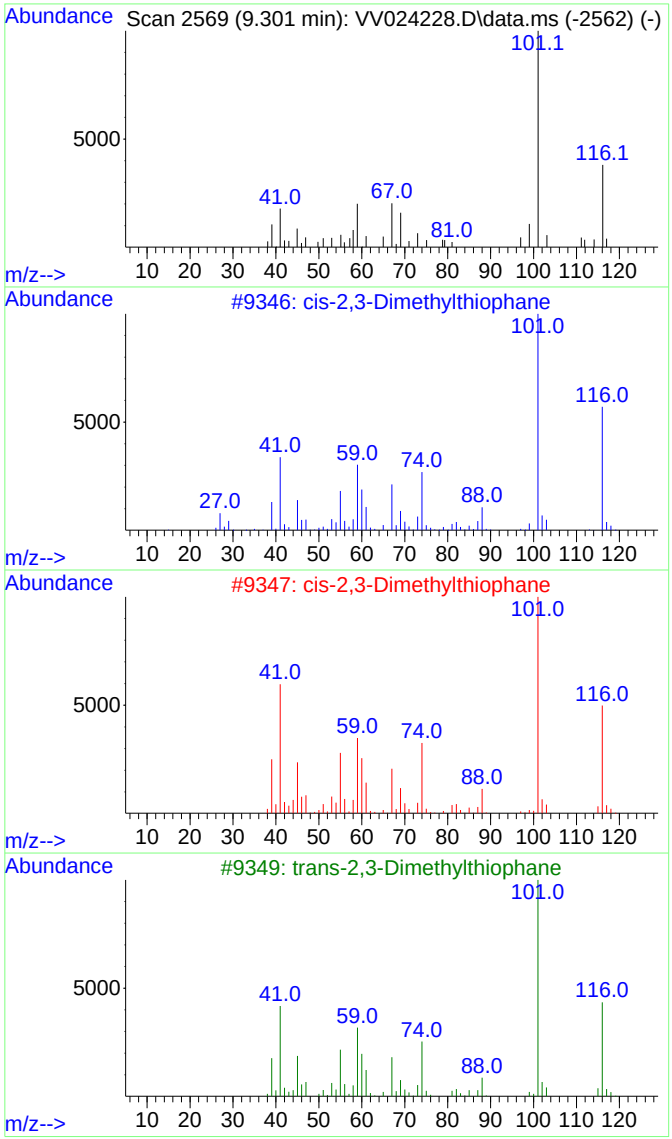
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR122721WMA.M
Quant Title : TRACE VOA SFAM1.0

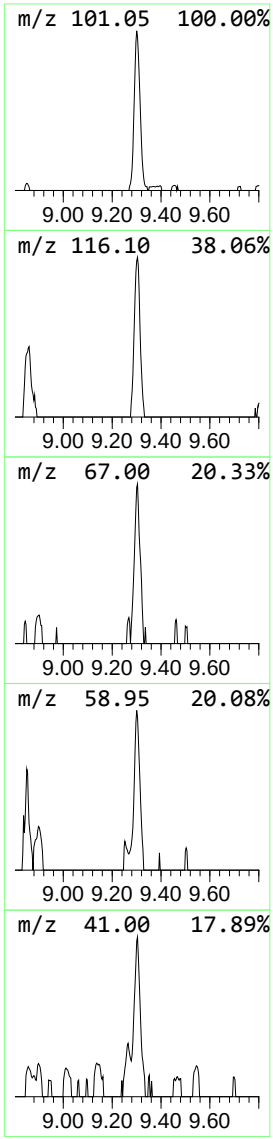
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 cis-2,3-Dimethylthiophane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.301	0.67 ug/L	32858	Chlorobenzene-d5	8.854

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-2,3-Dimethylthiophane	116	C6H12S	005161-77-3	64
2	cis-2,3-Dimethylthiophane	116	C6H12S	005161-77-3	64
3	trans-2,3-Dimethylthiophane	116	C6H12S	005161-78-4	53
4	Allylthiourea	116	C4H8N2S	000109-57-9	53
5	Thiazole, 4,5-dihydro-4-methyl-2...	116	C4H8N2S	010416-81-6	52





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV122821\
Data File : VV024228.D
Acq On : 28 Dec 2021 19:10
Operator : SY/MD
Sample : M5233-11DL2 100X
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
GBCC9DL2

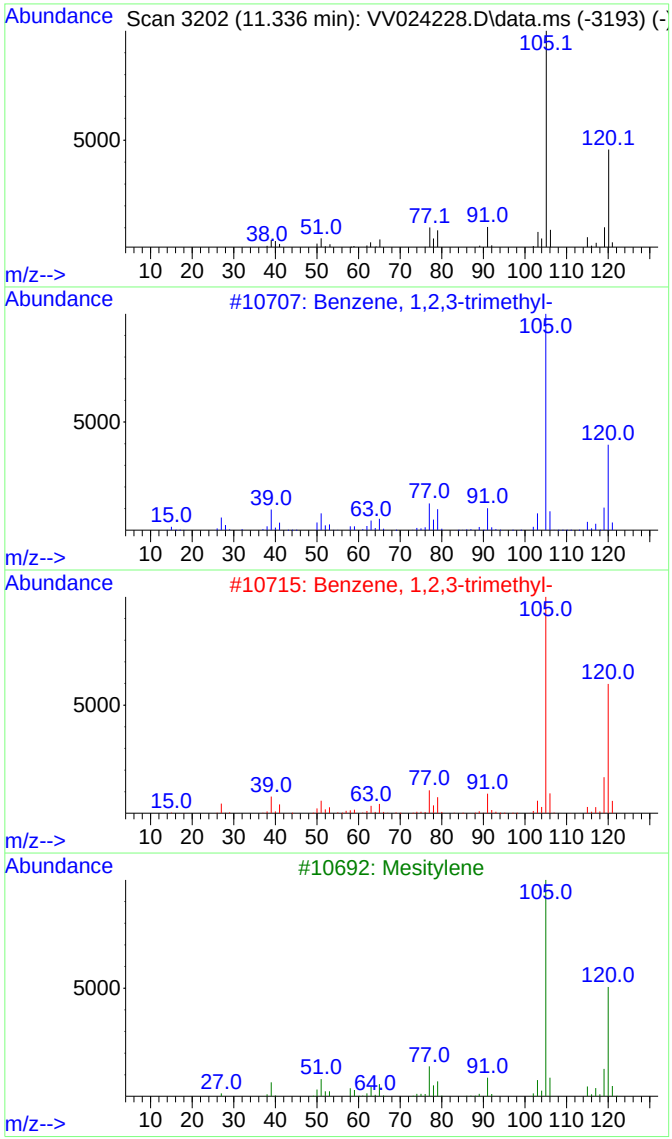
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR122721WMA.M
Quant Title : TRACE VOA SFAM1.0

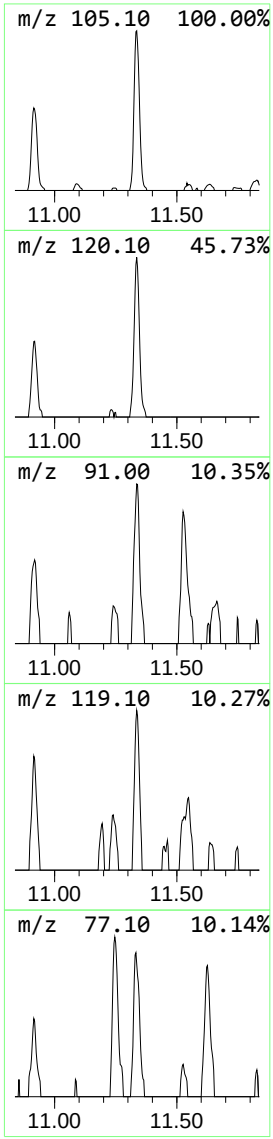
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 1-ethyl-4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.336	0.71 ug/L	35203	1,4-Dichlorobenzene-d4	11.249

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	97
2	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
3	Mesitylene	120	C9H12	000108-67-8	94
4	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
5	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV122821\
Data File : VV024228.D
Acq On : 28 Dec 2021 19:10
Operator : SY/MD
Sample : M5233-11DL2 100X
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
GBCC9DL2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR122721WMA.M
Quant Title : TRACE VOA SFAM1.0

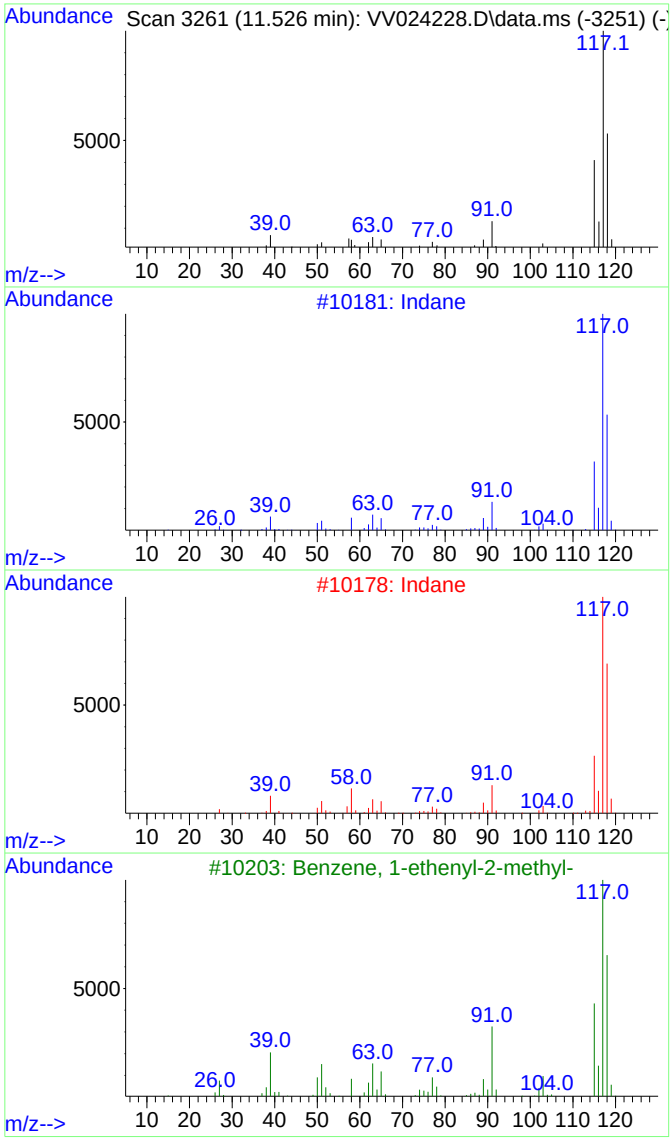
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

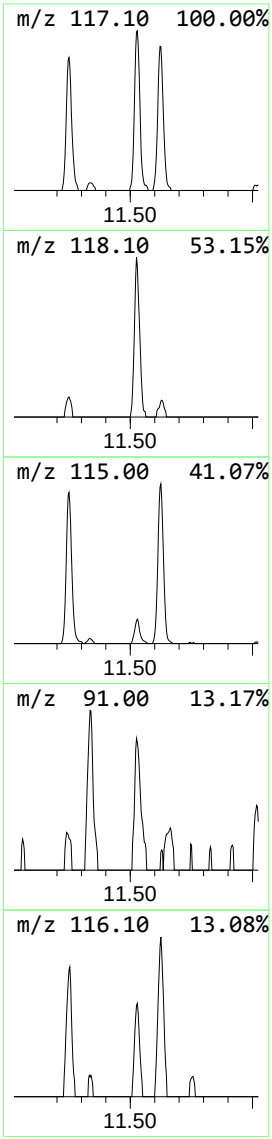
****

Peak Number 10 Indane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.525	0.55 ug/L	27415	1,4-Dichlorobenzene-d4	11.249

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	81
2	Indane	118	C9H10	000496-11-7	68
3	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	62
4	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	58
5	Benzene, 1-propenyl-	118	C9H10	000637-50-3	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV122821\
Data File : VV024228.D
Acq On : 28 Dec 2021 19:10
Operator : SY/MD
Sample : M5233-11DL2 100X
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
GBCC9DL2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR122721WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
(DEL) Alkane: S...	1.214	1.1	ug/L	41139	1	5.616	180269	5.0
Aminomethanesul...	1.417	5.0	ug/L	181194	1	5.616	180269	5.0
(DEL) Alkane: C...	1.819	0.6	ug/L	23234	1	5.616	180269	5.0
(DEL) Alkane: C...	1.902	0.5	ug/L	18162	1	5.616	180269	5.0
(DEL) Alkane: C...	2.024	2.1	ug/L	74398	1	5.616	180269	5.0
Cyclopentene	2.481	1.1	ug/L	38099	1	5.616	180269	5.0
cis-2,3-Dimethy...	9.301	0.7	ug/L	32858	2	8.854	245486	5.0
Benzene, 1-ethy...	11.336	0.7	ug/L	35203	3	11.249	248034	5.0
Indane	11.525	0.6	ug/L	27415	3	11.249	248034	5.0